

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property  
Organization  
International Bureau



(43) International Publication Date  
8 January 2004 (08.01.2004)

PCT

(10) International Publication Number  
WO 2004/003683 A2

- (51) International Patent Classification<sup>7</sup>: G06F
- (21) International Application Number: PCT/US2003/019905
- (22) International Filing Date: 26 June 2003 (26.06.2003)
- (25) Filing Language: English
- (26) Publication Language: English
- (30) Priority Data: 60/392,372 1 July 2002 (01.07.2002) US
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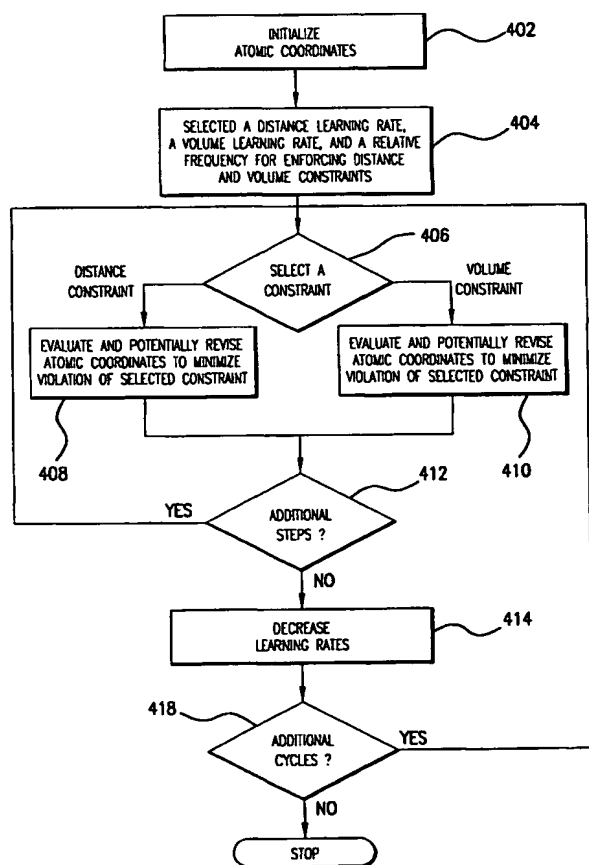
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(81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

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(54) Title: CONFORMATIONAL SAMPLING BY SELF-ORGANIZATION



(57) Abstract: A self-organizing method, system, and computer program product for generating molecular conformations that are consistent with a set of distance and/or volume constraints. A stochastic proximity embedding (SPE) algorithm evaluates individual distance and/or volume constraints and adjusts the atomic coordinates to minimize violations of such constraints. The method scales linearly with the number of atoms, and produces many more unique conformations at a fraction of the time required by conventional distance geometry algorithms.

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